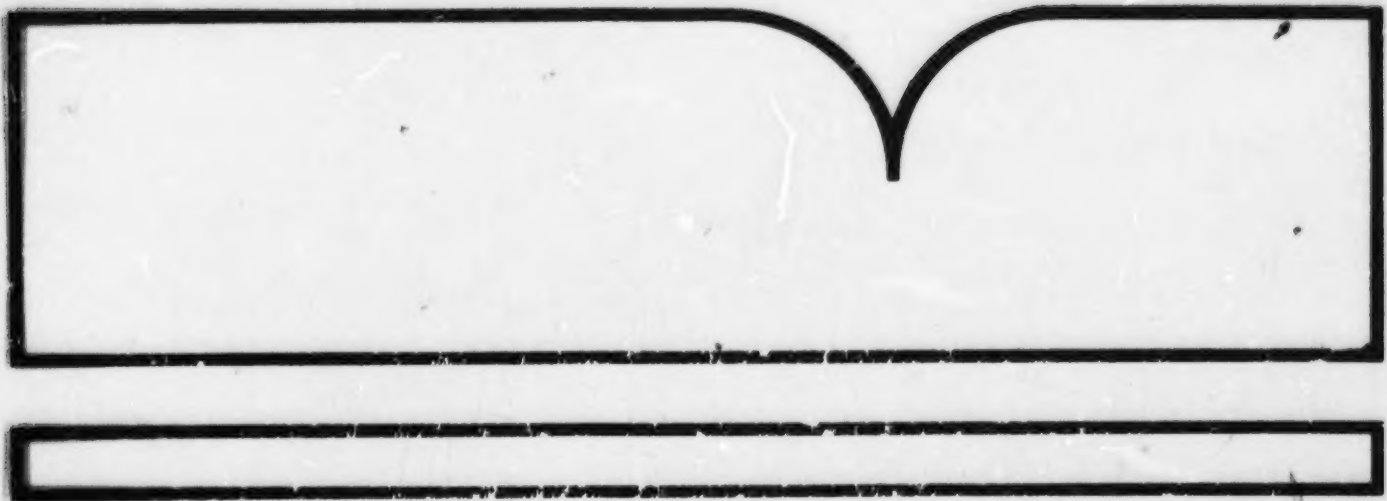


Statistical Considerations in the Employment of
Sax (Scanning Electron Microscopy with Automated
Image Analysis and X-Ray Energy Spectroscopy)
Results for Receptor Models

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STATISTICAL CONSIDERATIONS IN THE EMPLOYMENT OF SAX RESULTS FOR
RECEPTOR MODELS

by

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Hundreds of thousands of individual particle measurements may be accumulated in a receptor model study employing Scanning electron microscopy with Automated image analysis and X-ray energy spectroscopy (SAX). At present, the summaries of these data are utilized in apportionment calculations. Two basic approaches have been taken to the sorting of these observations: variable algorithms which are sample specific, and fixed algorithms which have temporal and inter-airshed continuity. We report here the use of a "fixed" sorting scheme developed for one area as it is applied to an airshed where no source specific information was available. Discriminant analysis, as applied to the individual particle characterizations, was shown to be very useful in improving the quality of the mathematical solution using a Q mode Factor/Vector analysis. It is concluded that statistical manipulation of the individual object vectors is more efficient than dealing with data summaries. Use of a "fixed" sorting algorithm is shown to be feasible when unknown ambient aerosol samples are to be apportioned to sources on the basis of their comparison with library "source signatures."

Introduction

Scanning Electron Microscopy (SEM) and Analytical Light Microscopy (ALM) techniques, as applied to aerosol samples, can extract much valuable information from the heterogeneous nature of individual particle assemblages. Utilized along with traditional receptor models such as the CMB, they improve source resolution. In fact, given appropriate sample collection and/or preparation, microscopy-based analytical methods of individual particle characterization present viable alternatives to bulk chemical analysis models. Scanning electron microscopy interfaced with Automated image analysis and X-ray energy spectroscopy (SAX) methods create and store hundreds or thousands of object vectors from the aerosol particles of each sample obtained¹. General descriptions of the methodology can be found in the works of Johnson², Hanna et al³, Johnson et al⁴, Casuccio and Janocko⁵, McIntyre et al⁶, and Johnson and McIntyre⁷; therefore we will not present any operational details of the technique here. Instead, we will concentrate on the problems of, and approaches to, sorting and classifying the individual particle analytical data for use in SAX receptor models.

If SAX characterizations of aerosols could be absolute, with unique identification of each particle coming from a particular source, then the model would be absolute and no further manipulation of the results would be required. But sources are variable and SAX suffers certain inherent limitations⁸ which preclude it from being quantitative (for a given particle) at the present time. Therefore, practitioners of this technique must employ summaries of the data which result from some sorting or classification scheme. No doubt some information is lost in this compression of the observations, so it is important to examine the applicability of the two major approaches to particle classification and subsequent data use.

Currently SAX observations are sorted by either a "fixed" or a "variable" algorithm (we mean these in a generic sense). In the "fixed" case, two major approaches are taken. In a linear file structure, the user defines the number of categories desired with chemical and physical specifications for each. An object vector (particle with certain morphological and relative X-ray intensity chemical observations) is sifted through the file until it comes to the category for which it meets all the requirements. The other alternative for the "fixed" file structure is to sift the particle using best-fit criteria for the defined classification structure⁹.

A "variable" sorting algorithm builds classes of particles from the object vector data of the sample. It may employ a relative X-ray intensity "ranked clustering" approach to identify unique groups of particles. Thus the classifications and the resulting data summaries may be different in structure from sample to sample. Results from a "variable" sorting algorithm are employed in the mathematical aspects of receptor models in a different way than are those of "fixed" schemes. "Variable" sorting results are used in a "Fingerprint/Ratio" receptor model¹⁰. "Tracer" particle types from specific sources are identified in ambient aerosol samples and their dilution ratios fitted by a least squares procedure to estimate source contributions. Such an approach has the specific advantage of higher information entropy¹¹, since unused classes are not reported, and it shows excellent resolution of sources. However, it requires that airshed-specific source information be available. That is, ambient samples may contain "tracer" classes of particles which are not recognized as such since no source analyses pointed them out and were identified with them. Thus, the "variable" sorting algorithm and the Fingerprint/Ratio SAX receptor model are difficult to apply to airshed aerosol collections which are depauperate in specific source samples.

The "fixed" sorting algorithm takes a more generalized approach in SAX receptor models. A fixed classification scheme for all ambient and source sampling allows a long term (or historic) internal consistency in the comparing of results. In this sense it is more like a bulk chemical analysis - library source signatures can be applied to receptor models for airsheds in which little or no source information is available. This approach is a cost effective preliminary receptor model for source apportionment, and used along with bulk analysis, can increase the resolution of CMB models.

Of course, there are disadvantages in the blanket of a "fixed" particle classification scheme. What is optimum for one airshed may not be for another. In this report we show how statistical treatment of the SAX observation vectors can improve the source apportionment of an unknown airshed when employing "library source signatures." The specific example is that of discriminant analysis of Houston aerosols to optimize their classification. This report represents an advance in interpretation over that presented at the Quail Roost II Conference.

Methods

SAX analyses of aerosol samples were carried out on 25 coarse fraction samples of Houston aerosol collected by dichotomous sampler on Nuclepore® membrane filters during September of 1980. A detailed description of sample collection and background history can be found in Dzubay *et al*¹² and in the Quail Roost II report by Stevens *et al*¹³. We have chosen 4 samples from this set of 25 upon which to base our examples of object vector manipulation. Table I lists the filter identifications and the sampling times for the 4 samples considered here, and presents the results of the original SAX

TABLE I. Houston Nuclepore Filters used in Experiment. Times and dates of collection and original SAX analyses for population and weight are shown.

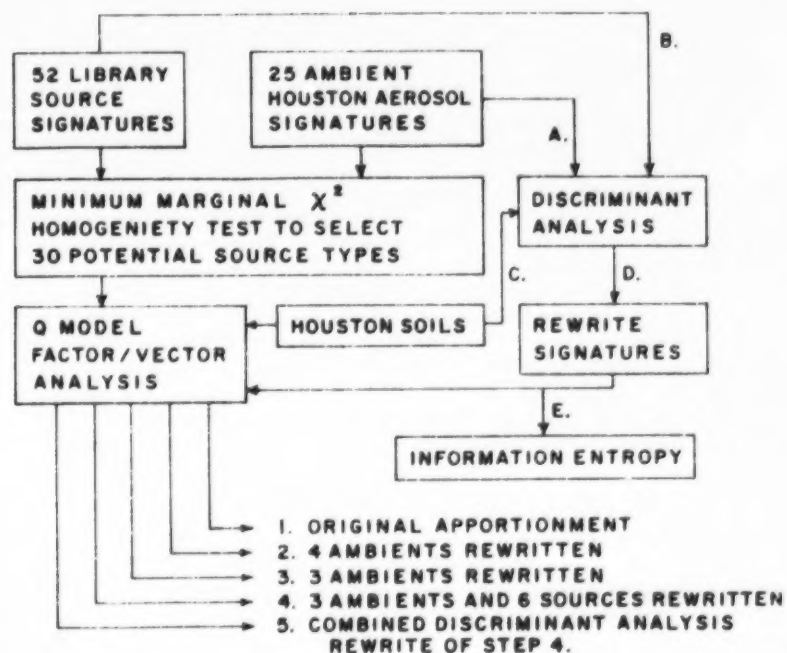
	124-502C		124-510C		124-516C		124-522C	
	9/10/80	7am	9/12/80	7pm	9/14/80	7pm	9/16/80	7pm
Particle Class	#%	Wt%	#%	Wt%	#%	Wt%	#%	Wt%
1. Low counts	8.9	1.4	14.3	4.9	6.5	0.5	0.9	0
2. Marine	0	0	0	0	8.6	6.7	17.3	13.7
3. S only	0.3	0	0	0	0	0	0.4	0
4. Ca & S	2.0	2.5	2.6	2.7	2.5	1.2	1.5	0
5. Wood ash	0.5	1.5	0.6	1.2	0.2	0	0.4	0.2
6. Refuse ash	0.9	0.3	0.1	0	0	0	0.2	0
7. Auto	3.6	3.1	4.8	1.8	3.6	4.8	4.3	1.1
8. Oil FA	0	0	0.4	0.7	0.6	0.2	0	0
9. Fly Ash, lg.	1.5	3.3	0.4	2.0	0.4	3.4	0	0
10. Fly Ash, sm.	4.4	1.2	7.1	2.5	6.3	2.2	2.8	1.1
11. Metal Rich	11.8	6.7	2.6	0.6	3.0	2.3	2.8	0.9
12. Mg-Ca	0.3	0.4	0.3	0.1	0.8	0.5	0.9	0.3
13. Ca only	19.6	17.2	19.3	42.8	30.3	32.0	36.6	60.3
14. Construction	7.0	12.7	5.0	4.5	4.4	10.1	5.4	3.4
15. Talc like	1.0	0.1	0.8	0.6	0.2	0	0	0
16. Illite like	0.1	0.2	0.3	0	0.4	0.3	0	0
17. Kaolinite like	2.5	0.5	1.7	0.8	1.1	0.1	0.2	0
18. Feldspar like	0	0	0	0	0	0	0.2	0
19. Biotite like	0	0	0	0	0	0	0	0
20. Muscovite like	1.1	1.5	2.1	2.2	1.5	1.9	0.6	1.1
21. Al rich	0.6	0.4	0.4	0	0	0	0	0
22. Si only	5.6	10.7	5.5	3.0	3.0	2.9	1.3	1.0
23. Misc. Litho.	20.6	32.6	22.5	25.0	16.0	25.3	13.4	7.8
24. Misc. Salts	2.6	0.4	2.7	2.7	4.2	0.7	3.2	2.1
25. Unknown	5.2	3.3	6.2	2.6	6.3	5.0	7.8	7.1

classification (population percent and weight percent) as determined by the "fixed" sorting algorithm employed for analysis of all source

and ambient samples.

All of the apportionment experiments carried out for this work have used the same mathematical treatment of the data - namely the Q-Model Factor/Vector analysis as described by Johnson and McIntyre⁷ from the work of Full et al¹⁴. Having selected a set of 33 possible source signatures from our signature library, which might reasonably apply to Houston aerosol, we have carried out a series of signature modification experiments to assess the efficiency of the original particle classifications. We wished to know how well source signatures from a "world list" could be applied to an unknown ambient aerosol using a "fixed" sorting algorithm. The signature library contained non-size fractionated SAX weight percent results for 52 sources (mostly from Syracuse, N.Y.) and 3 Houston Soil samples or road dusts. By using a Chi Square Minimum Marginal Homogeneity test¹⁵, 30 sources (types) were selected as potential end members for the Q-Model Factor/Vector analysis. These 30, along with the 3 Houston soils and the 25 ambient samples, were used consistently in the Q-Model apportionments. The experiments consisted of adjusting some of the signatures as described below. Figure 1 shows a block diagram for how these experiments were conducted.

The Q-Model apportionment is based upon a vector description of the position of the ambient samples within the extreme boundaries of sample space. The particular extremes (potential source types) might not be appropriate for the Houston airshed; yet they might allow a mathematically correct solution for the apportionment. We are not using the Factor Analysis portion of Q-Model as the sole mechanism for choosing the source types which go into the apportionment. Chi Square Minimum Marginal Homogeneity was employed to select those signatures from our library which might reasonably represent, in some mixture, the Houston aerosol. The test employs an $\chi \log \chi$ transformation of the number percent or weight percent by particle type categories (according to Kullback¹⁶). The 25 ambient samples were compared one at a time to each of the 52 library signatures and a homogeneity value calculated. The marginal or by-particle-class, contributions to the total homogeneity were computed. Any library source signature for which the cumulative marginal χ^2 homogeneity for 2/3 of the 25 particle class types was less than the critical value (95% confidence level) was retained for inclusion in the Q-Model apportionment calculations. Certain generic signatures (5 in all) were also retained; these included: secondary particles, sea salt, calcium sulfate, limestone, and organic debris.



- A. AMBIENTS: -502, -510, -516, -522 DISCRIMINATED INDIVIDUALLY
 B. SOURCES: 6 LISTED IN TABLE III DISCRIMINATED INDIVIDUALLY
 C. HOUSTON SOIL 1: DISCRIMINATED INDIVIDUALLY
 D. DISCRIMINATED SIGNATURES REWRITTEN FROM NUMBER PERCENT TO WEIGHT PERCENT - SEE TEXT
 E. INFORMATION ENTROPY CALCULATED FOR NEW SIGNATURES

Fig. 1. Flow diagram for the steps in the statistical manipulation of the SAX results.

The 4 example aerosol samples as well as 6 prominent "source" samples were subjected to discriminant analysis (avg. 500 object vectors, or particles, per sample) using SAS¹⁶ programs. Each particle object vector contained the nominal or original linear chemistry definition file classification, the image area, the total net x-ray count for the particle, and the relative x-ray intensity for up to 22 elements. These were punched on cards (approximately 5250 total) for creation of a SAS data set which could also be used for Factor and Cluster analyses.

After discriminant analysis for each sample of 500 particles, the discriminant functions indicated some reclassification of the original object vectors. From the discriminated results, a new weight percent by-particle-class signature was created and substituted in the Q-Model run to see how it affected the apportionments. The new weight percent signatures were created from the discriminated set of object vectors using the image area, assuming that each particle was spherical, and utilizing the specific gravity assigned to the particle type⁷. The "efficiency" of the restructured signatures was evaluated by the information entropy approach of Pull et al¹¹. Shannon¹⁸ defined entropy in the following fashion:

$$E = - \sum_{i=1}^n P_i \log P_i$$

where P_i is the probability of finding an observation in class i and n is the number of classes in the sorting algorithm (25 in this work). Entropy, as applied to either the number percent or weight percent by particle class histograms, is a measure of the contrast between classes. The entropy of the "fixed" classification scheme is a measure of the potential of the signature histograms to provide reasonable solutions when further analysis is performed on that set of summary data.

Figure II contains the original results of the SAX procedure as well as the discriminant analysis results for ambient sample 124-502C as a histogram of the original weight percent by particle class signature along with the new signatures that were created by the discriminant procedure. The classes, by number, are those given in Table 1. The classification procedure provided by the discriminated particle data is advantageous as it places each particle in a class by its best fit. In the original procedure, the particle must meet strict requirements before being placed in a certain class. The miscellaneous class percentage is reduced by the discriminant procedure and class thirteen (limestone) is increased. The two histograms for 124-502C have only slight differences and yet the percent of maximum possible information entropy is increased. The discriminant procedure is also advantageous as it uses all the information provided by the analysis to make a classification.

Results and Discussion

Q-model Factor/Vector analysis was used as an apportionment tool for this series of investigations. We have operated it in a

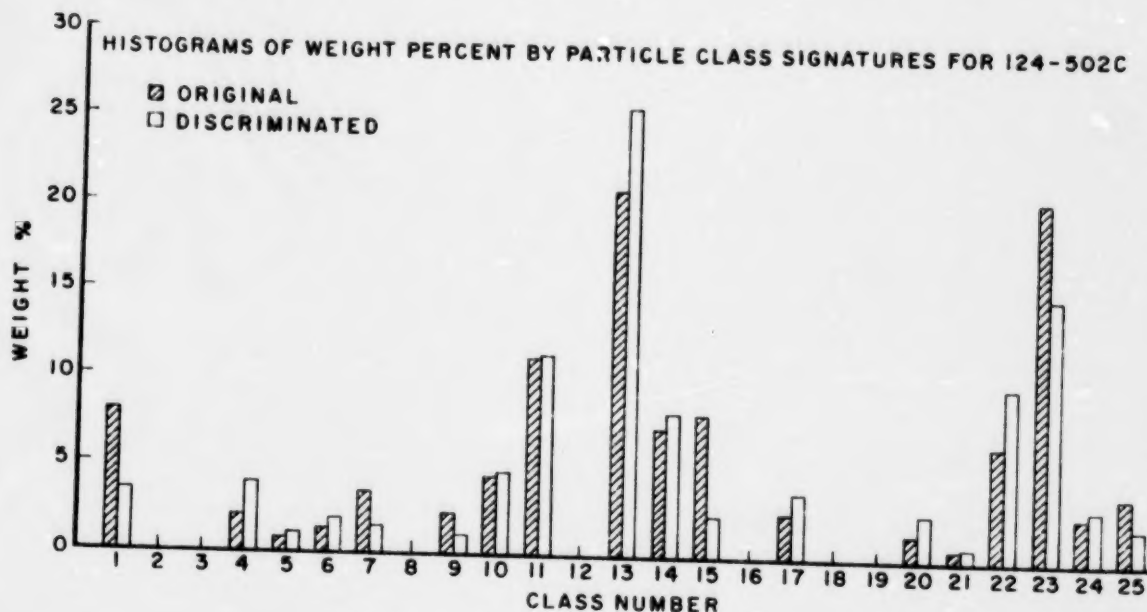


Fig. 2. Original and adjusted Signature.

manner, with the same set of source signatures and ambient sample signatures, so that our results are internally consistent. Our purpose was to adjust the "signatures" of certain ambient and source samples, after statistical manipulation of the object vectors, in order to judge whether the refinements improve or worsen the apportionment results. Reclassification of original observations, by discriminant analysis, leads to a restructuring of the "signatures" used in an apportionment model. This process implies an increase in information "entropy" which means more efficient use of the data

contained in the summaries object vector characterizations. However, the drive towards maximum information entropy leads toward the minimum in source resolution. Maximum information entropy for a "fixed" number of categories would be obtained by an equal distribution of observations in each of the possible classes. Maximum source resolution would result from unique classification in one of the possible particle type categories. Both resolution and information entropy can be increased by increasing the number of classes in the categorization scheme. However, "counting statistics" for maximum precision would then dictate more data acquisition for the sample. All these tendencies must be balanced at some optimum intermediate value of categories. At present, that number would seem to be between 15 and 20.

The use of a "fixed" sorting algorithm allows one to compare source signatures from a library against the analysis results for samples from an unknown airshed. We have assumed that a classification scheme developed for one region will not be optimum when applied to another region. Our "fixed" chemistry definition file for particle sorting was developed on the basis of "standard" materials from the Syracuse AQMA. When individual particles (object vectors) from several samples were subjected to discriminant analysis, we found that 15% of them were reclassified. That is, our step functions in the linear sorting algorithm were only 85% optimum. When Houston aerosol object vectors were sifted with the same scheme and subjected to discriminant analysis, we found a 30% reclassification rate on a sample by sample basis. Since the "fixed" file structure was only 70% optimum for Houston aerosol, the question arose, "How reasonable are the apportionment results for Houston based on library source signatures?"

It would seem that if classification schemes are not optimum, there is a high probability that the apportionment mathematics employed are also not optimally efficient. There is much value in examining the negative apportionment vectors - especially when library signatures are to be applied in a case where airshed-specific source information is lacking. Study of the negative apportionment vectors can reveal some structure of the potential sources. In operating Q-Model, after signature modification, we have employed two criteria for assessing optimum data treatment: we have looked at the change in information entropy after signature adjustment, and we have examined the sum of the negative apportionment vectors in the common case where we specified a 12 end member (potential source) solution.

Q-Model begins with a factor analysis of the samples and observation variables submitted to it. For a particular run or application there may be different dimensionalities to the

mathematical solution of the vector analysis depending upon variance of the input data. When utilizing the 58 entries for this work, we decided to cut off the number of factors (end members) at the point where the eigen values fell below 1.00. This resulted in the specification of a 12 end member (factor) solution, and explained 95% of the variability in the complete data set. The Q-Model computations were carried out with summaries of the SAX data (weight percent by particle class histograms). When the individual object vectors were subjected to factor analysis (500 at a time), higher degrees of dimensionality were indicated. The number of factors seemed to be related to the number of elements monitored by the X-ray spectrometer. When unusual, or trace, elements like I, Sn, Cd, Mo, and Se were eliminated from the variables for factor analysis, 10-12 factors routinely had eigen values greater than 1.00. Thus, all Q-Model experimental runs were made using 12 possible end members (factors identified with specific sources). Table II shows the "initial" and "final" source apportionment results for the Houston aerosol samples which we studied in detail.

TABLE II. Comparison of Initial and Final Q-Model Source type fractional apportionments for three Houston aerosol samples.*

Source Type	124-502C		124-510C		124-516C	
	Init.	Final	Init.	Final	Init.	Final
Coal FA 1	.50		.56		.34	
Coal FA 2	-.10		-.10		-.05	
Steel Mill	-.13	.05	-.20	-.01	-.12	0
Limestone	.06		.26		.21	
Sea Salt	.01	0	.02	.01	.06	.05
Cement Plant	.01	.09	.01	.62	0	.37
Organic Debris	.03	0	.05	.01	.02	0
Auto (Pb)	.05	.01	.05	-.01	.06	.04
CaSO ₄	.09	.05	.10	.03	.06	.03
Construction	.54	.49	.33	.15	.43	.35
2° Particles	.01	0	.01	-.01	.01	0
Dirt 1 (Syr)		-.03		.03		-.01
HST Soil 2		.37		.29		.21
Misc.	-.07	-.02	-.08	-.09	-.02	-.03

* Initial apportionments as submitted to Q-Model. Final apportionments after discriminant analysis reclassification for three ambient and six source signatures.

The signature readjustment experiments were conducted by within-sample discriminant analysis in a series of steps. Step 1 was the Q-Model apportionment carried out on the original signatures. In

Step 2, four of the Houston ambient aerosol samples were discriminated individually and the resulting adjusted (or best fit) particle class population signatures converted to weight percent by particle class histograms for substitution in the Q-Model apportionment. In Step 2, Houston ambient sample 124-522 was selected as a potential source type after discriminant analysis and signature rewrite. Therefore, in Step 3, sample 124-522 was eliminated from the Q-Model run. In Step 4, six of the prominent potential source type signatures were discriminated, rewritten, and subjected to the Q-Model apportionment as replacements for the existing signature entries. In the final step of the experiment, Number 5, all of the individual particle object vectors were simultaneously subjected to discriminant analysis for signature rewrite and inclusion in the Q-Model apportionment.

Table III shows the general success (or non-success) of the discriminant analysis prior to Q-Model apportionments. What is displayed is the summation of the negative apportionment vectors for each step of the experiment as outlined above. Also shown (in parentheses) are the calculated information entropy values as a percentage of the maximum possible for the original and rewritten signatures. The values presented are for the rewritten weight percent-by-particle class signatures.

It would appear from these results that a generic or source type apportionment of unknown ambient aerosol samples can be made using a source type signature library and employing SAX methods. From an examination of the emission inventory for the Houston AQMA, the types of apportionments shown in Table II would appear reasonable. Of course, the approach utilized here is dependent upon the textural quality of the source type signature library - potential major source types must be on file. In the case of the Houston aerosol samples used in this example, the apportionment results indicate that much of the aerosol has calcium rich sources (cement plant like, construction/destruction, limestone, and CaSO_4). Based upon this type of SAX apportionment, it would seem that subsequent source samplings (as may be required in Houston) should concentrate on appropriate Ca rich sources.

It can be seen from the example results for Step 5 (Table III) that as information entropy increases, resolution of source types decreases. Clearly the application of discriminant analysis to the individual object vectors within a sample of aerosol material can sharpen the signature histograms which result from SAX characterizations. This helps to circumvent the difficulty of not having an "optimum" sorting scheme for each airshed. As long as the source signature library contains the minimum of appropriate signature types, best-fit manipulation of the raw SAX data would seem to show

great promise in generic source apportionments of unknown samples.

TABLE III. Summary of total negative apportionment vectors.

[STEPS]	1	2	3	4	5
Sample	Original	New Ambients	New Ambients [▲] (Not 552)	All New Signs.* (Not 522)	Total Discrim. [‡]
124-502C	-30.4 (63)**	-19.9	-19.3	-5.9	-7.7 (80)
124-510C	-37.2 (56)	-31.7	-25.4	-12.6	-25.5 (62)
124-516C	-19.5 (62)	-14.4	-14.6	- 4.9	114.0 (70)
124-522C	- 3.5	0	- 6.8	-23.8	

▲ Sample 124-522 chosen as "extreme" in step 2. Did not use Discrim. Signature in later steps.

* New Discrim. signatures for 502, 510, 516, Limestone, Syracuse Dirt 7, Foundary Sand, Houston Soil 1, Lime Kiln, Coal fly ash 2.

‡ New Discrim. signatures, as in step 4, but all 9 signatures submitted to the same discriminant analysis calibration simultaneously.

** Percentage of maximum possible information entropy.

There are some limitations in the use of SAX data for source apportionment. One particular problem is when the individual particle being characterized is an aggregate, possibly representing particle emission for several sources. Such particles obviously exist in nature but no quantified description in ambient aerosol is apparent. Through the use of multiple source samplings and through "features" in the SEM image, the presence of aggregates can be determined. These particles can be divided among two or more categories, or eliminated for consideration in the statistical summary of the total sample. In the case of the results we present here, software limitations precluded these options as the x-rays collected were from the geometric center of the particle feature. Manual quantification of

the sample we used indicated a low incidence of compositionally distinct aggregates. We feel, therefore, that the characterization of large numbers of particles (greater than 600) in each specimen will tend to average out the uncertainties. Further work is needed to quantify this SAX model uncertainty.

Conclusions

SAX analyses of unknown aerosol samples can be used in a generic receptor model apportionment scheme which utilizes a library of source type signatures. "Fixed" particle type sorting algorithms developed for one airshed may not be optimum when applied to other airshed ambient samples. However, the results of the experiments performed here with the raw analytical data for individual particle observations show that the quality of the mathematical solution can be improved to acceptable levels. Unknown ambient aerosol samples, characterized by SAX methods, can be apportioned by using a "world list" of source type signatures. The results can serve as a guide to improving the resolution of CMB receptor models and can indicate where source sampling efforts can be most efficiently pursued. It is clear that statistical treatment of the raw data (object vectors for individual particles) is more efficient than dealing with the summaries of such observations.

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